Gas diffusion layer reconstruction and fuel cell modeling

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Summary

Fuel cells (FCs) are devices that convert chemical energy to electricity and have the theoretical potential to operate at very high efficiency, while they are environmentally friendly since there are no pollutant emissions. A lot of research has been dedicated to the development of efficient and sustainable FC devices and significant progress has been made. However, there are still some issues that need to be resolved in order for this technology to be widely used. One of the main drawbacks is the relatively high cost of this technology, necessitating strong efforts by researchers and technological companies to develop more efficient and inexpensive materials for the FC components and to address degradation and durability issues. Water and heat management issues present strong research interest since they affect dramatically the cell durability. A key FC component to water management is the Gas Diffusion Layer (GDL) inasmuch as its structure and properties can lead to effective removal of the produced water and prevent cell flooding.

In this work the GDL structure is computer-aided reconstructed and the GDL permeability is investigated for the cases of gas mixtures and two phase flow taking into account water evaporation/condensation during the process. Moreover, single FC operation is modeled and the role of different material properties and operation conditions is investigated.

For this purpose, a stochastic reconstruction algorithm for the GDL reconstruction has been developed. The algorithm utilizes information acquired from SEM pictures of GDL samples and data from the manufacturer, including relevant carbon fiber dimensions, teflon, PTFE and binder content and porosity. The algorithm accounts

also for the compression effect on the GDL during the assembling of FC stacks. Diffusivity and permeability calculations for gas flow are provided for different GDL structures. The compression effect on the transport properties of the material has been investigated in both through and in plane directions. Moreover, two phase flow inside the GDL has been modeled, including condensation and evaporation of water. Simulations were run for different operation parameters in order to identify the conditions, structural properties and operational parameters, to prevent or limit water condensation and subsequent GDL flooding. GDL hydrophobicity or hydrophilicity has also been considered. In addition, a single-FC 3D model has been developed that accounts for compressible flow and transport of species including convection and diffusion, electrochemical reactions and current distribution, as well as heat production and transfer. A number of different material properties and operation parameters effect FC efficiency. The actual geometry of a single FC, especially the thickness of its components and the gas channel topology, can also have considerable impact on the FC performance. The single-FC model has been used to investigate the impact of different material properties, operation conditions and geometries. These results can be used together with experimental data as guidelines for the improvement of material properties and operation conditions so that more efficient fuel cells can be designed and constructed.